Final Progress Report (4/15/05 to 9/30/08)

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Project Name: Validation and Enhancement of Computational Fluid Dynamics and Heat Transfer Predictive Capabilities for Generation IV Reactor Systems

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A) Executive Summary

Nationwide, the demand for electricity due to population and industrial growth is on the rise. However, climate change and air quality issues raise serious questions about the wisdom of addressing these shortages through the construction of additional fossil fueled power plants. In 1997, the President's Committee of Advisors on Science and Technology Energy Research and Development Panel determined that restoring a viable nuclear energy option was essential, and that the DOE should implement a R&D effort to address principal obstacles to achieving this option. This work has addressed the need for improved thermal/fluid analysis capabilities, through the use of computational fluid dynamics, which are necessary to support the design of Generation IV gas-cooled and supercritical water reactors.

The methodology implemented involved both experimental and computational work. In particular, experiments were performed for a number of fundamental geometries to provide validation data for the computational fluid dynamics methodologies. These included both the Reynolds averaging approach (RANS), and a large eddy simulation (LES) approach. The results indicated that the RANS approach was able to predict the experimental data to within levels that could be considered suitable for engineering calculations. More difficulties were encountered with the LES approach when heat transfer was an important consideration in determining the resulting flow.

B) Comparison Between Accomplishments and Original Goals/Objectives

RANS Modeling Activities

The goals of the project involved the completion and assessment of calculations for 1) Shehata/McEligot tube data; 2) parallel jet calculations; 3) jet in cross flow within a cylinder array. The results for the Shehata/McEligot tube data were successfully completed and published in Refs [1, 2, 3] below. The parallel jet calculations (within an infinite array) have been completed, and are awaiting final experimental data before being published at a meeting conference. The jet in cross flow within cylinder calculations have been completed, and presented in Refs. [4, 5, 6]. The results of these calculations are presented in somewhat greater detail below.

LES Modeling Activities

The goals of the project involved the completion and assessment of calculations for 1) Shehata/McEligot tube data; 2) parallel jet calculations. Some of the results for the Shehata/McEligot tube data were published in Refs [7, 8] below. The parallel jet calculations (within an infinite array) have been postponed because we have performed more simulations on the Shehata/McEligot tube, since wall temperature prediction is strongly dependent on the grid resolution/choice. We are currently also looking into a Direct Numerical Simulation to be able to better evaluate the LES model shortfalls.

Experimental Activities

Our original goals were to measure parallel heated jets, and flow through a cylinder array with cross flow. The cross flow was eliminated (since this experiment had been performed by INL) and these measurements were shifted to an air facility at USU. The heated parallel jets were measured as planned. The INL experiment was changed to swirling jets. The MIR facility made it possible to use a prescribed hard-wall boundary condition while still obtaining optical data. These results have been published in Refs. [9-12]

C) Summary of Project Activities

RANS Modeling Activities

Assessment of a Second-Moment Closure for Strongly Heated Internal Gas Flows

Both low- and high-Reynolds-number versions of the $stress - \omega$ model of Wilcox were used to predict velocity and heat transfer data in a high-heat-flux cylindrical tube for which fluid properties varied strongly with temperature. The results indicate that for accurate heat transfer calculations under the conditions considered in this study, inclusion of low-Reynolds-number viscous corrections to the model are essential. The failure of the high Reynolds number model to accurately predict the wall temperature was attributed to an over prediction of the near-wall velocity.

Turbulence Model Assessment for Flow Across a Row of Confined Cylinders

The effectiveness of five different turbulence models is assessed for the flow across a row of confined cylinders at a pitch-to-diameter ratio of 1.7, and at Reynolds numbers ranging from 2621 to 55920. Models examined include the one-equation Spalart-Almaras model, two-equation realizable $k - \varepsilon$, $k - \omega$, and shear stress transport (SST) models, and a four-equation $v^2 - f$ model. Quantities compared against published experimental data include minor loss coefficients, separation angles about cylinders, wake lengths behind cylinders, and streamwise velocity profiles at the periodic inlet/outlet boundaries. Results indicate that each of the models did a reasonable job in predicting the minor loss coefficient as a function of Reynolds number. With the exception of the $k - \varepsilon$ model, each was also able to predict the experimentally observed trend of decreasing wake and separation lengths with increasing Reynolds number. In addition, all models also predicted a local minimum in the separation angle about the inner cylinder as a function of Reynolds number, which has also been observed experimentally. Our conclusion is that the $v^2 - f$ model performed slightly better at predicting the experimental data than any of

the other models examined, although at the computational expense of solving two additional equations.

Infinite Array of Parallel Jets

The steady, Reynolds-averaged Navier-Stokes equations are solved for an infinite array of isothermal jets using $k - \varepsilon$, $k - \omega$, $v^2 - f$, and *stress* - ω turbulence models. The jets are arranged in an equilateral triangular grid such that the spacing between jet centers is 2D, where D is the jet diameter at the exit plane. The jets develop as they pass through a smooth contraction (of radius D) in a plate of thickness D. This inlet geometry produces a jet at the exit plane which contains a significant potential core region. In terms of the calculations, symmetry conditions are imposed to minimize the extent of the computational domain to the extent that ¹/₄ sections of two adjacent jets are employed. In that sense, an infinite array of jets differs from a single jet in that, due to symmetry considerations, the net entrainment of fluid into the jets from the quiescent surroundings is zero. Model results at a Reynolds number of 850 will be compared against experimental data of Smith et al. at downstream locations z/D=0, 1, 2, and 4. The results have not yet been published.

LES Modeling Activities

LES simulations were performed to predict the Shehata/McEligot experiments for the "low" heating rate case with an inlet Reynolds number of approximately 6000. Results computed using several LES subgrid models to experimental results, and to results obtained using the Reynolds Averaged Navier-Stokes RANS approach. In our work we compare the following four subgrid-scale stress (SGS) models:

Smagorinsky-Lilly (SL)

Smagorinsky-Lilly Dynamic (SLD)

Wall-Adapting Local Eddy-Viscosity (WALE)

Kinetic-Energy Transport (KET)

One simulation run of the full pipe geometry with 600,000 grid points takes about 30 days of computation. These simulations use the Vortex and Spectral Synthesizer turbulence generation methods implemented in Fluent at the inlet. All simulations under-predicted the average wall temperature. An overview over the simulations performed is given in Table 1:

Turbulence generation method at inlet	SGS model	Pressure discretization method
Vortex	SL	2 nd order
Vortex	SLD	2 nd order
Vortex	KET	2 nd order
Vortex	WALE	2 nd order
Spectral Synthesizer	SL	2 nd order
Spectral Synthesizer	SLD	2 nd order
Spectral Synthesizer	KET	2 nd order

Table 1: Full length heated pipe simulations.

Spectral Synthesizer	WALE	2^{nd} order
Spectral Synthesizer	WALE	PRESTO

In order to better evaluate the influence of grid resolution a large number of simulations on shorter geometries were performed. Most of these simulations over-predict the wall temperature compared to the $v^2 - f$ model. An overview over these simulations is given in table 2 and 3.

Table 2: Short pipe runs - 5D length with square center grid for performance comparisons to other, non-square center grids. All simulations were run using the WALE SGS model with both turbulence generation techniques at the inlet, Vortex method and Spectral Synthesizer (SS). These cases under-predict the wall temperature.

#of pts in theta dir	#of points in r dir	spacing in z direction
		(m)
80	25	0.0015
80	25	0.0025
80	25	0.0035
96	24	0.0015
96	24	0.0025
96	24	0.0035
112	23	0.0015
112	23	0.0025
112	23	0.0035

Table 3: Short pipe runs - 10D with cylindrical grid to test grid convergence. All models were run to convergence using both Vortex and SS methods. These simulations over predict the wall temperature.

#of pts in theta dir	#of points in r dir	spacing in z dir (m)
100	40	0.0025
100	40	0.0035
100	48	0.0025
100	48	0.0035
130	40	0.0025
130	40	0.0035
130	48	0.0025

In order to evaluate the influence of the model constant C_s , LES simulations with changes of the constant (see Table 4) were performed, but no significant influence on the results were observed.

Table 4: Short pipe run - 10D to evaluate WALE model using SS, with 130 pts in theta direction, 48 in z dir, and z spacing of 0.0025 m (finest grid).

Value of C_s constant
0.162
0.244
0.325 (default)
0.406
0.650

Currently, a set of simulations is under way where the inflow of the LES simulation is generated by using a periodic pipe simulation.

Experimental Activities

Cylinder Array Data

These data were fully acquired and published. The results of assessment of various turbulence models based on these data were also published.

Our conclusions: This experiment was undertaken primarily to determine the variation of flow regime versus Reynolds number for a confined row of short cylinders simulating some aspects of flows in the lower plenum of a typical GCR design and to examine whether useful guidance is provided by existing data for large arrays of long circular cylinders. Stream wise central cylinders and wall-mounted half-cylinders formed an equilateral triangular pattern with P/D about 1.7 and H/D about 7. Reynolds numbers, based on minimum flow area and cylinder diameter, ranged from about 240 to 56,000. Measurements included pressure drop per row and PIV data for instantaneous and mean velocity fields plus related mean statistics. For the third cylinder and beyond, the flow was approximately stream wise periodic. The PIV fields were obtained away from the side-walls in the central region where the flow was essentially two dimensional in the mean. The loss coefficients are somewhat below the graphical correlations of Žukauskas for Reynolds numbers between 3000 and 56,000. The detailed PIV results permitted categorizing the flow into five regimes in contrast to the three suggested by Žukauskas.

These regimes are as follows:

- 1. steady laminar flow, Re < 398
- 2. unsteady laminar flow, 444 < Re < 507
- 3. mixed, partially turbulent flow, 597 < Re < 1858
- 4. mixed turbulent flow, Re < 2621

5. turbulent flow, none of the present cases are conclusively in this regime those employed in computer turbulence models. We recommend using LES or at least unsteady Reynolds-averaged Navier-Stokes RANS codes when attempting to predict these measurements.

Parallel Heated Jet Data

This experiment proved very problematic. In order to get sufficient heating in the jets, the flow speeds were low enough that very small room currents had an effect. This may render the data unsuitable for turbulence model assessment. The results have not been published.

Swirling Jet Data

Since the cylinder array data was acquired in USU facilities, our effort in the INL MIR facility was changed to measurements of jets including high degrees of swirl. In this experiment, generality is sacrificed for the sake of precise boundary conditions. The jets issued into a large, quartz tube ensuring that the boundary condition could be well-described. A very detailed set of measurements has been obtained and will be presented at the 2009 ICONE meeting in Brussels.

D) Products Developed

Publications

1. Spall, R.E., Nisipeanu, E., and Richards, A., "Assessment of a Second-Moment Closure Model for Strongly Heated Internal Gas Flows," *Journal of Heat Transfer*, Vol. 129, pp. 1719-1722, 2007.

2. Spall, R.E., Nisipeanu, E., and Richards, A., "Assessment of a Second-Moment Closure Model for Strongly Heated Internal Gas Flows," ASME-JSME Thermal Engineering Summer Heat Transfer Conference, July 8-12, 2007, Vancouver, BC.

3. Richards, A.H., Spall, R.E., "Simulation of Strongly Heated Internal Gas Flows Using a Near-Wall Two-Equation Heat Flux Model," ICONE14-89808, International Conference on Nuclear Engineering, Miami, FL, July 17-20, 2006.

4. Hodson, J, Spall, R.E., and Smith, B.L., "Turbulence Model Assessment for Flow Across a Row of Confined Cylinders," Nuclear Technology, Vol. 161, pp. 268-276, 2008.

5. Hodson, J.D., Spall, R.E. and Smith, B.L. "RANS Predictions in an Idealized Lower-Plenum Model," 14th International Conference on Nuclear Engineering, July, 2006. Paper ICONE14-89222.

6. Hodson, J., Thorson, E., Spall, R.E., and Smith, B.L., "CFD Validation of Flow Regimes in an Idealized Lower-Plenum Model," American Nuclear Society Winter Meeting and Technology Expo, 2005.

7. Hradisky, M., Hauser, T., Richards, A., and Spall, R.E., "Large Eddy Simulation of Strongly Heated Internal Gas Flows," AIAA-2006-3260, 9th AIAA/ASME Joint Thermophysics and Heat Transfer Conference, San Francisco, California, June 5-8, 2006

8. Hradisky, M. & Hauser, T. Evaluating Les Subgrid-Scale Models for High Heat Flux Flows ASME-JSME Thermal Engineering and Summer Heat Transfer Conference, 2007

9. Smith, B.L., Stepan, J.J., and McEligot, D., "Velocity And Pressure Measurements Along A Row Of Confined Cylinders," J. Fluids Eng. Vol. 129, pp.1314-1327, 2007.

10. Stepan, J.J., and Smith, B.L. "Time-Resolved 3-Component Velocity Measurements of an Array of Heated Jets," Bull. Am. Phys. Soc. 52, 2007.

11. Spall, R.E., Smith, B.L., Richards, A.H., and McEligot, D.M., "Numerical and Experimental Analysis of Turbulent Flow Along a Rod Bundle," American Nuclear Society Winter Meeting, Albuquerque, NM, November 12-16, 2006.

12. Smith, B.L., Thorson, E.V., and McEligot, D., "Flow Field Measurements Along a Row of Confined Cylinders," Bull. Am. Phys. Soc. 50, pg. 81, 2005.

13. Wilson, B., Smith, B., and Spall, R.E., "Turbulence Model Assessment for a swirling jet with high swirl number" International Conference on Nuclear Engineering, paper ICONE17-75362, 2009.

E) Computer Modeling

No new computer codes were developed under this project. The commercially available computational fluid dynamics code FLUENT was used for all numerical simulations. The code is well documented on the web site www.fluent.com.